Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssptansc1625

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	OCT 02	CA/CAplus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 3	OCT 19	BEILSTEIN updated with new compounds
NEWS 4	NOV 15	Derwent Indian patent publication number format enhanced
NEWS 5	NOV 19	WPIX enhanced with XML display format
NEWS 6	NOV 30	ICSD reloaded with enhancements
NEWS 7	DEC 04	LINPADOCDB now available on STN
NEWS 8	DEC 14	BEILSTEIN pricing structure to change
NEWS 9	DEC 17	USPATOLD added to additional database clusters
NEWS 10	DEC 17	IMSDRUGCONF removed from database clusters and STN
NEWS 11	DEC 17	DGENE now includes more than 10 million sequences
NEWS 12	DEC 17	TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS 13	DEC 17	MEDLINE and LMEDLINE updated with 2008 MeSH vocabulary
NEWS 14	DEC 17	CA/CAplus enhanced with new custom IPC display formats
NEWS 15	DEC 17	STN Viewer enhanced with full-text patent content from USPATOLD
NEWS 16	JAN 02	STN pricing information for 2008 now available
NEWS 17	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS 18	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS 19	JAN 28	MARPAT searching enhanced
NEWS 20	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS 21	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS 22	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS 23	FEB 08	STN Express, Version 8.3, now available
NEWS 24	FEB 20	PCI now available as a replacement to DPCI
NEWS 25	FEB 25	IFIREF reloaded with enhancements
NEWS 26	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS 27	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 18:40:49 ON 11 MAR 2008

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 18:41:03 ON 11 MAR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5
DICTIONARY FILE UPDATES: 10 MAR 2008 HIGHEST RN 1007341-18-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

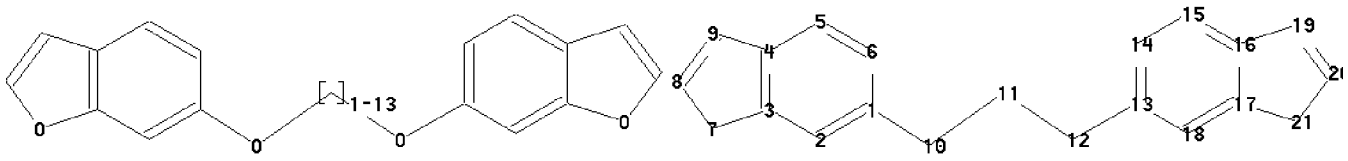
TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10507925.str



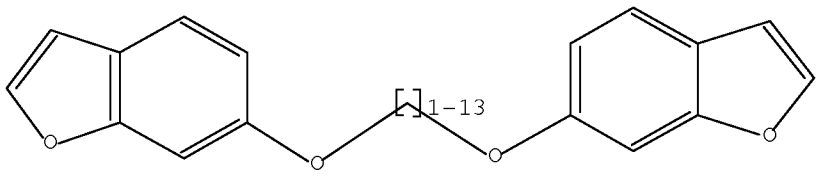
chain nodes :
10 11 12
ring nodes :
1 2 3 4 5 6 7 8 9 13 14 15 16 17 18 19 20 21
chain bonds :
1-10 10-11 11-12 12-13
ring bonds :
1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9 13-14 13-18 14-15 15-16 16-17

16-19 17-18 17-21 19-20 20-21
exact/norm bonds :
1-10 3-7 4-9 7-8 8-9 10-11 11-12 12-13 16-19 17-21 19-20 20-21
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom

L1   STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1   STR



Structure attributes must be viewed using STN Express query preparation.

=> s sss l1 sam
SAMPLE SEARCH INITIATED 18:41:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   1280 TO ITERATE

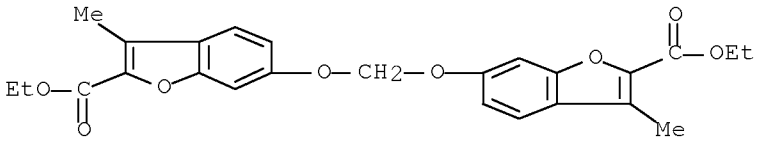
100.0% PROCESSED   1280 ITERATIONS   1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 23454 TO   27746
PROJECTED ANSWERS: 1 TO   80

L2   1 SEA SSS SAM L1

=> d scan

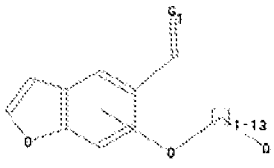
L2   1 ANSWERS   REGISTRY COPYRIGHT 2008 ACS on STN
IN   2-Benzofurancarboxylic acid, 6,6'-[methylenebis(oxy)]bis[3-methyl-,
     diethyl ester (9CI)
MF   C25 H24 O8

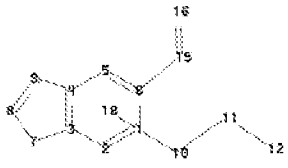


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=>
Uploading C:\Program Files\Stnexp\Queries\10507925B.str





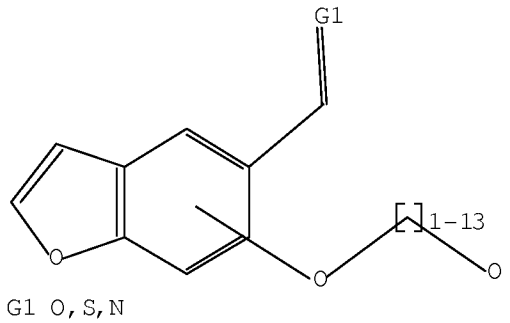
chain nodes :
10 11 12 15 16
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
6-15 10-11 11-12 15-16
ring bonds :
1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9
exact/norm bonds :
3-7 4-9 7-8 8-9 10-11 11-12 15-16
exact bonds :
6-15
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 15:CLASS 16:CLASS 18:Atom

L3 STRUCTURE UPLOADED

=> D L3
L3 HAS NO ANSWERS
L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> S SSS L3 SAM
SAMPLE SEARCH INITIATED 18:55:45 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 14700 TO ITERATE

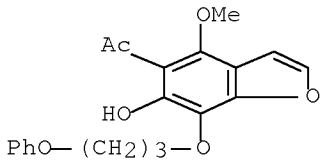
13.6% PROCESSED 2000 ITERATIONS 1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 286737 TO 301263
PROJECTED ANSWERS: 1 TO 309

L4 1 SEA SSS SAM L3

=> D SCAN

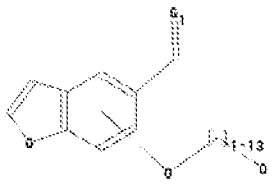
L4 1 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Ethanone, 1-[6-hydroxy-4-methoxy-7-(3-phenoxypropoxy)-5-benzofuranyl]-
MF C20 H20 O6

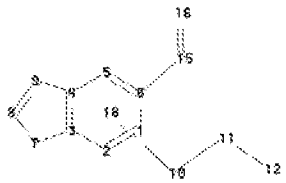


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=>
Uploading C:\Program Files\Stnexp\Queries\10507925C.str





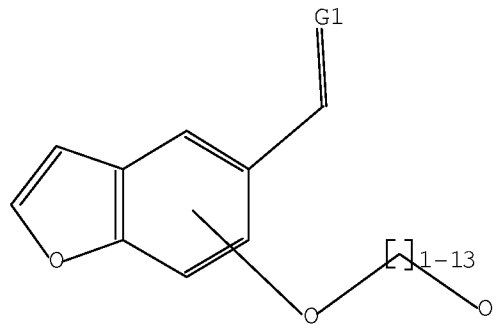
chain nodes :
10 11 12 15 16
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
6-15 10-11 11-12 15-16
ring bonds :
1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9
exact/norm bonds :
3-7 4-9 7-8 8-9 10-11 11-12 15-16
exact bonds :
6-15
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 15:CLASS 16:CLASS 18:Atom

L5 STRUCTURE UPLOADED

=> D L5
L5 HAS NO ANSWERS
L5 STR



G1 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> S SSS L5 SAM
SAMPLE SEARCH INITIATED 18:58:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 14700 TO ITERATE

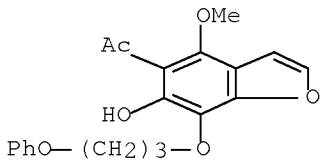
13.6% PROCESSED 2000 ITERATIONS 1 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 286737 TO 301263
PROJECTED ANSWERS: 1 TO 309

L6 1 SEA SSS SAM L5

=> D SCAN

L6 1 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Ethanone, 1-[6-hydroxy-4-methoxy-7-(3-phenoxypropoxy)-5-benzofuranyl]-
MF C20 H20 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> S SSS L5 FULL

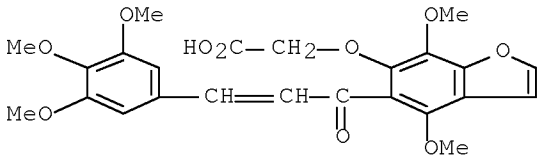
FULL SEARCH INITIATED 18:58:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 292385 TO ITERATE

100.0% PROCESSED 292385 ITERATIONS 125 ANSWERS
SEARCH TIME: 00.00.02

L7 125 SEA SSS FUL L5

=> D SCAN

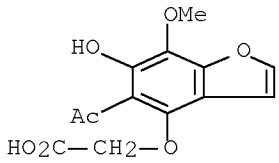
L7 125 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Acetic acid, [[4,7-dimethoxy-5-[1-oxo-3-(3,4,5-trimethoxyphenyl)-2-propenyl]-6-benzofuranyl]oxy]- (9CI)
MF C24 H24 O10



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

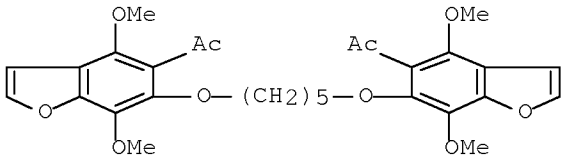
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L7 125 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Acetic acid, [(5-acetyl-6-hydroxy-7-methoxy-4-benzofuranyl)oxy]- (6CI, 9CI)
MF C13 H12 O7



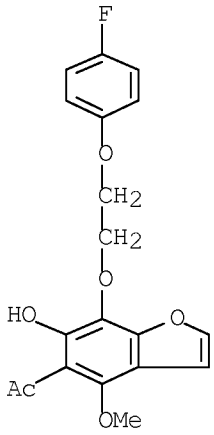
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 125 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Ethanone, 1,1'-[1,5-pentanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI)
MF C29 H32 O10



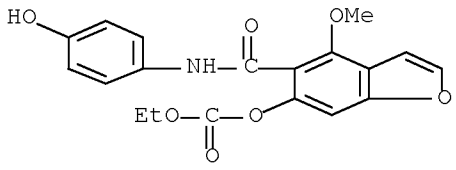
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 125 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Ethanone, 1-[7-[2-(4-fluorophenoxy)ethoxy]-6-hydroxy-4-methoxy-5-benzofuranyl]-
MF C19 H17 F O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L7 125 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Carbonic acid, ethyl 5-[[(4-hydroxyphenyl)amino]carbonyl]-4-methoxy-6-benzofuranyl ester (9CI)
MF C19 H17 N O7



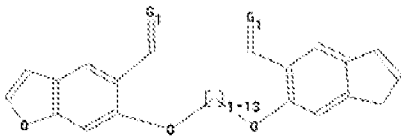
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

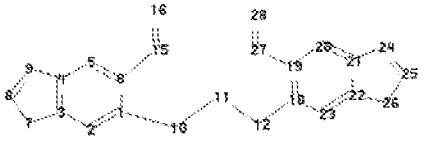
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> SAVE TEMP L7 BAEL/10507925/A
BAEL/10507925/A IS NOT A VALID SAVED NAME
Enter the name you wish to use for the saved query,
answer set, or L-number list. The name must:
1. Begin with a letter,
2. Have 1-12 characters,
3. Contain only letters (A-Z) and numbers (0-9),
4. End with /Q for a query (search profile, structure, or screen set), /A for an answer set, or /L for an L-number list.
5. Not already be in use as a saved name,
6. Not be END, SAV, SAVE, SAVED
7. Not have the form of an L-number (Lnnn).
ENTER NAME OR (END):END

=> SAVE TEMP L7 BAEL10507925/A
ANSWER SET L7 HAS BEEN SAVED AS 'BAEL10507925/A'

=>
Uploading C:\Program Files\Stnexp\Queries\10507925D.str





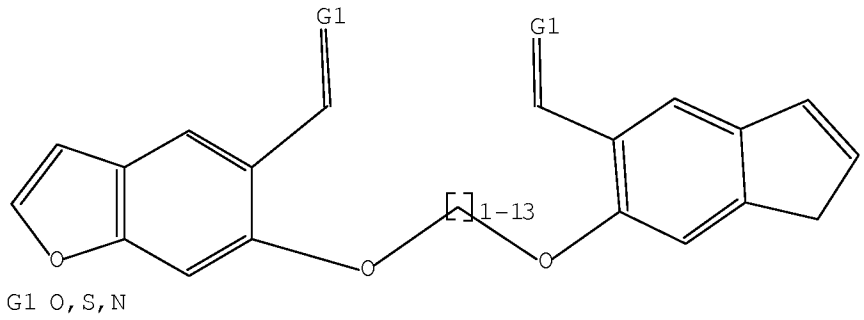
chain nodes :
10 11 12 15 16 27 28
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26
chain bonds :
1-10 6-15 10-11 11-12 12-18 15-16 19-27 27-28
ring bonds :
1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9 18-19 18-23 19-20 20-21 21-22 21-24 22-23 22-26 24-25 25-26
exact/norm bonds :
1-10 3-7 4-9 7-8 8-9 10-11 11-12 12-18 15-16 21-24 22-26 24-25 25-26 27-28
exact bonds :
6-15 19-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23

G1:O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 15:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 27:CLASS 28:CLASS

L8   STRUCTURE UPLOADED

=> D L8
L8 HAS NO ANSWERS
L8   STR



Structure attributes must be viewed using STN Express query preparation.

=> S SSS L8 SAM
SAMPLE SEARCH INITIATED 19:05:47 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   94 TO ITERATE

100.0% PROCESSED   94 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS: 1299 TO   2461
PROJECTED ANSWERS: 0 TO   0

L9   0 SEA SSS SAM L8

=> S SSS L8 SUBSET=L7 SAM
SAMPLE SUBSET SEARCH INITIATED 19:06:23 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED -   0 TO ITERATE

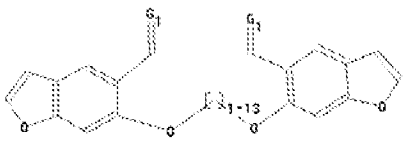
100.0% PROCESSED   0 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.01

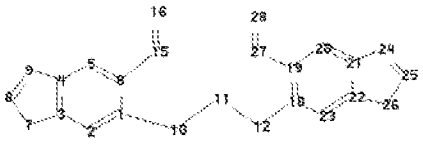
PROJECTIONS (WITHIN SPECIFIED SUBSET):   ONLINE **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):   0 TO   0
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):   0 TO   0

L10   0 SEA SUB=L7 SSS SAM L8

=> D SCAN
L10 HAS NO ANSWERS

=>
Uploading C:\Program Files\Stnexp\Queries\10507925E.str





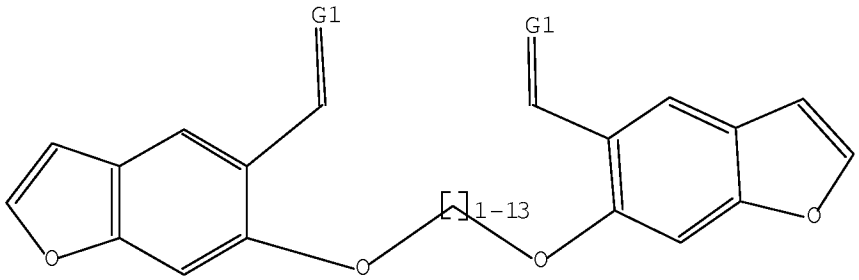
chain nodes :
10 11 12 15 16 27 28
ring nodes :
1 2 3 4 5 6 7 8 9 18 19 20 21 22 23 24 25 26
chain bonds :
1-10 6-15 10-11 11-12 12-18 15-16 19-27 27-28
ring bonds :
1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9 18-19 18-23 19-20 20-21 21-22
21-24 22-23 22-26 24-25 25-26
exact/norm bonds :
1-10 3-7 4-9 7-8 8-9 10-11 11-12 12-18 15-16 21-24 22-26 24-25 25-26
27-28
exact bonds :
6-15 19-27
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 18-19 18-23 19-20 20-21 21-22 22-23

G1:O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 15:CLASS 16:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom
25:Atom 26:Atom 27:CLASS 28:CLASS

L11 STRUCTURE UPLOADED

=> D L11
L11 HAS NO ANSWERS
L11 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> S SSS L11 SAM
SAMPLE SEARCH INITIATED 19:08:16 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      112 TO ITERATE

100.0% PROCESSED      112 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         1606 TO     2874
PROJECTED ANSWERS:               0 TO        0

L12           0 SEA SSS SAM L11

=> D HIS

     (FILE 'HOME' ENTERED AT 18:40:49 ON 11 MAR 2008)

     FILE 'REGISTRY' ENTERED AT 18:41:03 ON 11 MAR 2008
L1              STRUCTURE UPLOADED
L2            1 S SSS L1 SAM
L3              STRUCTURE UPLOADED
L4            1 S SSS L3 SAM
L5              STRUCTURE UPLOADED
L6            1 S SSS L5 SAM
L7          125 S SSS L5 FULL
                SAVE TEMP L7 BAEL10507925/A
L8              STRUCTURE UPLOADED
L9            0 S SSS L8 SAM
L10           0 S SSS L8 SAM SUB=L7
L11             STRUCTURE UPLOADED
L12           0 S SSS L11 SAM

=> S SSS L11 SUBSET=L7 SAM
SAMPLE SUBSET SEARCH INITIATED 19:09:07 FILE 'REGISTRY'
SAMPLE SUBSET SCREEN SEARCH COMPLETED -        0 TO ITERATE

100.0% PROCESSED        0 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):           ONLINE  **COMPLETE**
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PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET): 0 TO 0
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET): 0 TO 0

L13 0 SEA SUB=L7 SSS SAM L11

=>

=> S SSS L11 SUBSET=L7 FULL
FULL SUBSET SEARCH INITIATED 19:09:24 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 17 TO ITERATE

100.0% PROCESSED 17 ITERATIONS 5 ANSWERS
SEARCH TIME: 00.00.01

L14 5 SEA SUB=L7 SSS FUL L11

=> FIL CAPL
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 241.62 241.83

FILE 'CAPLUS' ENTERED AT 19:09:31 ON 11 MAR 2008
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FILE COVERS 1907 - 11 Mar 2008 VOL 148 ISS 11
FILE LAST UPDATED: 10 Mar 2008 (20080310/ED)

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=> S L14
L15 4 L14

=> D IBIB ABS HITSTR 1-4

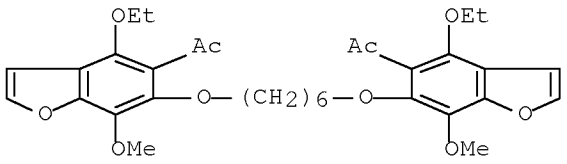
L15 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:87666 CAPLUS Full-text
DOCUMENT NUMBER: 144:331145
TITLE: A New Class of Blockers of the Voltage-Gated Potassium Channel Kv1.3 via Modification of the 4- or 7-Position of Khellinone
AUTHOR(S): Harvey, Andrew J.; Baell, Jonathan B.; Toovey, Nathan; Homerick, Daniel; Wulff, Heike
CORPORATE SOURCE: The Walter and Eliza Hall Institute, Medical Research Biotechnology Centre, Bundoora, 3086, Australia

SOURCE: Journal of Medicinal Chemistry (2006), 49(4), 1433-1441
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:331145

AB The voltage-gated potassium channel Kv1.3 constitutes an attractive target for the selective suppression of effector memory T cells in autoimmune diseases. We have previously reported the natural product khellinone, as a versatile lead mol. and identified two new classes of Kv1.3 blockers: (i) chalcone derivs. of khellinone, and (ii) khellinone dimers linked through the 6-position. Here we describe the multiple parallel synthesis of a new class of khellinone derivs. selectively alkylated at either the 4- or 7-position via the phenolic OH and show that several chloro, bromo, methoxy, and nitro substituted benzyl derivs. inhibit Kv1.3 with submicromolar potencies. Representative examples of the most potent compds. from each subclass, (5-acetyl-4-(4'-chloro)benzyloxy-6-hydroxy-7- methoxybenzofuran) and (5-acetyl-7-(4'-bromo)benzyloxy-6-hydroxy-4- methoxybenzofuran), block Kv1.3 with EC50 values of 480 and 400 nM, resp. Both compds. exhibit moderate selectivity over other Kv1-family channels and HERG, are not cytotoxic, and suppress human T cell proliferation at low micromolar concns.

IT 880479-06-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and voltage-gated potassium channel activity of khellinone analogs)

RN 880479-06-1 CAPLUS
CN Ethanone, 1,1'-[1,6-hexanediylbis[oxy(4-ethoxy-7-methoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:446728 CAPLUS Full-text
DOCUMENT NUMBER: 141:251728
TITLE: 1,6-Bis(5-acetyl-4,7-dimethoxybenzofuran-6-yloxy)hexane
AUTHOR(S): Baell, Jonathan B.; Gable, Robert W.; Harvey, Andrew J.
CORPORATE SOURCE: Structural Biology Chemistry Group, The Walter and Eliza Hall Institute of Medical Research, Biotechnology Centre, Bundoora, Victoria, 3086, Australia
SOURCE: Acta Crystallographica, Section E: Structure Reports Online (2004), E60(6), o996-o997
CODEN: ACSEBH; ISSN: 1600-5368
PUBLISHER: International Union of Crystallography
DOCUMENT TYPE: Journal; (online computer file)

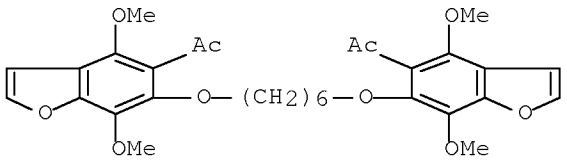
LANGUAGE: English

AB The khellinone dimer, 1,6-bis-(5-acetyl-4,7-dimethoxybenzofuran-6-yloxy)hexane, C30H34O10, was prepared as part of Kv1.3 ion channel blockers. Crystallog. data are given. The dimer lies on a center of symmetry, and adopts an extended structure such that the separation between the benzofuran groups is 9.927(3) Å. C-H···O H bonds link the mols. into linear chains which lie parallel to the [201] direction.

IT 605665-31-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

RN 605665-31-4 CAPLUS

CN Ethanone, 1,1'-[1,6-hexanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:178993 CAPLUS Full-text

DOCUMENT NUMBER: 140:375004

TITLE: Khellinone Derivatives as Blockers of the Voltage-Gated Potassium Channel Kv1.3: Synthesis and Immunosuppressive Activity

AUTHOR(S): Baell, Jonathan B.; Gable, Robert W.; Harvey, Andrew J.; Toovey, Nathan; Herzog, Tanja; Haensel, Wolfram; Wulff, Heike

CORPORATE SOURCE: Walter and Eliza Hall Institute of Medical Research Biotechnology Centre, Bundoora, 3086, Australia

SOURCE: Journal of Medicinal Chemistry (2004), 47(9), 2326-2336
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

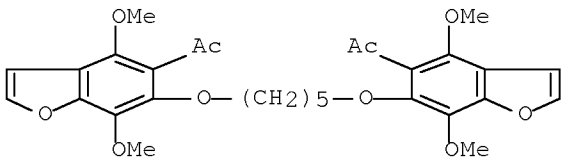
LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:375004

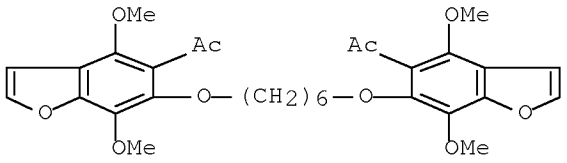
AB The voltage-gated potassium channel Kv1.3 constitutes a promising new target for the treatment of T-cell-mediated autoimmune diseases such as multiple sclerosis. In this study, we report the discovery of two new classes of Kv1.3 blockers based on the naturally occurring compound khellinone, 5-acetyl-4,7-dimethoxy-6-hydroxybenzofuran: (1) khellinone dimers linked via the alkylation of the 6-hydroxy groups and (2) chalcone derivs. of khellinone formed by Claisen-Schmidt condensation of the 5-acetyl group with aryl aldehydes. In particular, the chalcone 3-(4,7-dimethoxy-6-hydroxybenzofuran-5-yl)-1-phenyl-3-oxopropene and several of its derivs. inhibited Kv1.3 with Kd values of 300-800 nM and a Hill coefficient of 2, displayed moderate selectivity over other Kv1-family K+ channels, suppressed T-lymphocyte proliferation at submicromolar concns., and showed no signs of acute toxicity in mice. Because of their relatively low mol. weight and lipophilicity and their high affinity to Kv1.3, aryl-substituted khellinone derivs. represent attractive lead compds. for the development of more potent and selective Kv1.3 blocking immunosuppressants.

IT 605665-30-3P 605665-31-4P 605665-32-5P
684278-39-5P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and immunosuppressive activity of khellinone derivs.)

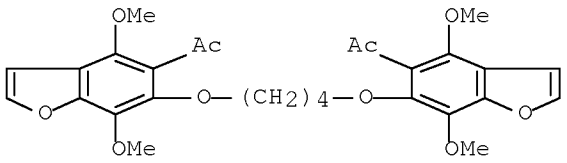
RN 605665-30-3 CAPLUS
CN Ethanone, 1,1'-[1,5-pentanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



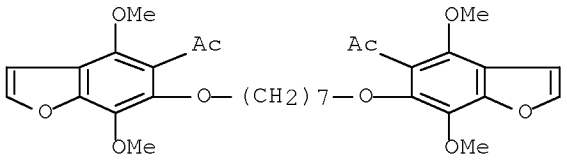
RN 605665-31-4 CAPLUS
CN Ethanone, 1,1'-[1,6-hexanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



RN 605665-32-5 CAPLUS
CN Ethanone, 1,1'-[1,4-butanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



RN 684278-39-5 CAPLUS
CN Ethanone, 1,1'-[1,7-heptanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:757693 CAPLUS Full-text
DOCUMENT NUMBER: 139:276752
TITLE: Preparation of divalent ligands based on khellinone derivatives as therapeutic ion channel blocking agents
INVENTOR(S): Baell, Jonathan B.; Wulff, Heike; Harvey, Andrew J.; Norton, Raymond S.; Chandy, George K.
PATENT ASSIGNEE(S): The Walter and Eliza Hall Institute of Medical Research, Australia
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003078416	A1	20030925	WO 2003-AU351	20030320
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2479481	A1	20030925	CA 2003-2479481	20030320
AU 2003212101	A1	20030929	AU 2003-212101	20030320
EP 1490349	A1	20041229	EP 2003-707912	20030320
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1656087	A	20050817	CN 2003-811505	20030320
JP 2005525384	T	20050825	JP 2003-576422	20030320
IN 2004DN02795	A	20070420	IN 2004-DN2795	20040920
US 2005261301	A1	20051124	US 2005-507925	20050705

PRIORITY APPLN. INFO.: AU 2002-1272 A 20020320
WO 2003-AU351 W 20030320

OTHER SOURCE(S): MARPAT 139:276752
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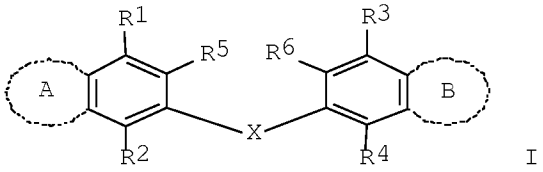

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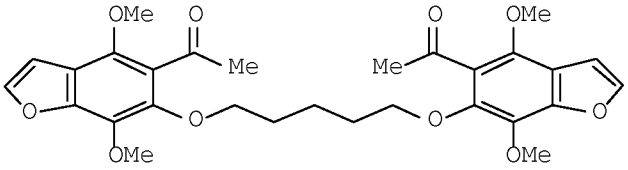
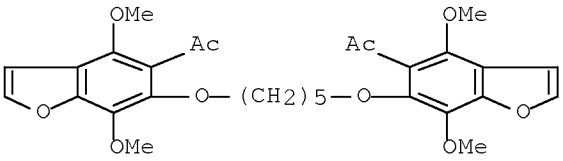


II

AB The title compds. [I; R1-R4 = H, OH, alkyl, alkoxy, etc.; X = a divalent spacer group that provides a spacing between the two aromatic rings to which it is joined of from 6 to 11 atoms when measured across the shortest route between the two aromatic rings; A, B = fused rings independently selected from (un)substituted 5-7 membered (hetero)aromatic and non-aromatic heterocyclic rings; R5, R6 = COR7, C(NR7)R7, CSR7 (R7 = H, alkyl, alkoxy, OH); with the proviso] which can be useful in the modulation of potassium channel activity in cells, including among others Kv1.3 channels found in T-cells, were prepared Thus, reacting khellinone with 1,5-dibromopentane in the presence of cesium carbonate in DMF afforded 65% II which showed Kd of 0.82 μM (Kv1.3) and Kd of 1.5 μM (Kv1.2). The compds. I may also be useful in the treatment or prevention of autoimmune and inflammatory diseases, including multiple sclerosis. Pharmaceutical composition comprising the compound I was claimed.

IT 605665-30-3P 605665-31-4P 605665-32-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of divalent ligands based on khellinone derivs. as therapeutic ion channel blocking agents)

RN 605665-30-3 CAPLUS
CN Ethanone, 1,1'-[1,5-pentanediylbis[oxy(4,7-dimethoxy-6,5-benzofurandiyl)]]bis- (9CI) (CA INDEX NAME)



RN 605665-31-4 CAPLUS
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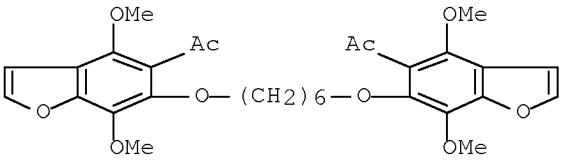

RN 605665-32-5 CAPLUS
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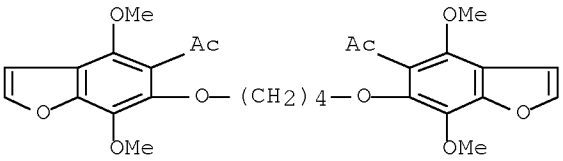

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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